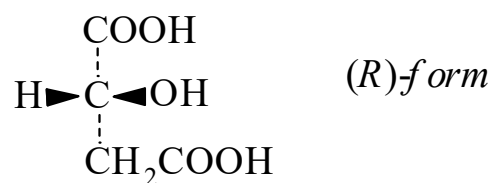




>>Entry Name: Malic acid, 8CI

ENTRY UNDER REVIEW

Synonym(s): Hydroxybutanedioic acid, 9CI. Hydroxysuccinic acid. E296. FEMA 2655



CAS Registry Number: 6915-15-7

Related CAS Registry Numbers(s): 149-61-1 676-46-0 3105-51-9 4387-09-1 22138-22-3 39015-77-5 68303-40-2

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>

Molecular Weight: 134.088

Accurate Mass: 134.021525

Percentage Composition: C 35.83%; H 4.51%; O 59.66%

Use/Importance: Flavour enhancer and other uses in food

Other Data: See (±)-form for food use

Hazard & Toxicity: Skin and severe eye irritant

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 636-61-3

Molecular Formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>

Molecular Weight: 134.088

Accurate Mass: 134.021525

Percentage Composition: C 35.83%; H 4.51%; O 59.66%

Biological Source: This enantiomer of rare occurrence; reported from fruits and leaves of *Hibiscus sabdariffa* although there are many more isolations of malic acid with no opt. rotn. given and some may be of the *R*-form

Physical Description: Cryst. (Et<sub>2</sub>O)

Melting Point: Mp 101° (97-99°)

Optical Rotation: [α]<sub>D</sub> +2.92 (MeOH). [α]<sub>D</sub><sup>20</sup> +28.4 (c, 5.5 in Py) (>99.8% ee)

Solubility: Sol. H<sub>2</sub>O, EtOH, Me<sub>2</sub>CO

pKa Value: pK<sub>a1</sub> 5.26 (25°, H<sub>2</sub>O)

Aldrich: 12241-6

Fluka: 2300

Sigma: M0750

Supelco: 4-6940

>>Derivative: Di-Na salt

CAS Registry Number: 138-09-0

Optical Rotation: [α]<sub>D</sub> +8.29 (H<sub>2</sub>O)

Sigma: M9138

>>Derivative: 1-Me ester

CAS Registry Number: 83540-94-7

Molecular Formula: C<sub>5</sub>H<sub>8</sub>O<sub>5</sub>

Molecular Weight: 148.115

Accurate Mass: 148.037175

Percentage Composition: C 40.55%; H 5.44%; O 54.01%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 79-80°

Optical Rotation: [α]<sub>D</sub><sup>20</sup> -5 (c, 9.5 in CH<sub>3</sub>OH)

>>Derivative: Di-Me ester

Synonym(s): Dimethyl malate